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14. ABSTRACT

We investigate the mechanisms of fatigue behavior in nano-crystalline metals at the atomic scale using empirical force laws and molecular level simulations. A combination of molecular statics and molecular dynamics was used to deal with the time scale limitations ofmolecular dynamics. We show that the main atomistic mechanism of fatigue crack propagation in these materials is the formation of nano-voids ahead of the main crack. The results obtained for crack advance as a functionof stress intensity amplitude are consistent with experimental studies and a Paris law exponent of about 2.

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ATOMISTIC MECHANISMS OF FATIGUE IN NANOCRYSTALLINE METALS.

AFOSR GRANT NUMBER F49620-03-1-0375

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Abstract

We investigate the mechanisms of fatigue behavior in nano-crystalline metals at the atomic scale using empirical force laws and molecular level simulations. A combination of molecular statics and molecular dynamics was used to deal with the time scale limitations of molecular dynamics. We show that the main atomistic mechanism of fatigue crack propagation in these materials is the formation of nano-voids ahead of the main crack. The results obtained for crack advance as a function of stress intensity amplitude are consistent with experimental studies and a Paris law exponent of about 2.

Research Objective

Fatigue of metallic materials is an important issue in the general field of mechanical behavior. In particular, nano-crystalline materials are particularly susceptible to fatigue failure [1,2]. This constitutes one of the limitations of this new class of metallic materials and the behavior can be generally attributed to the presence of a large fraction of grain boundary material. The details of fatigue failure mechanisms are not well understood. Theoretical models have been generally limited to the macroscopic and meso-scale and no studies have been performed at the atomistic level, to the best of our knowledge [3-6]. There are two basic reasons why fatigue has not been studied atomistically, relating to length scale and time scale. In the present work, we show that with current computing power, we can approach the experimental fatigue length scale of nm/cycle crack extension. The time scale is more problematic. The detailed mechanism by which plasticity affects crack advance is not precisely known and therefore there is no clear way to predict the effects of the unrealistic high cycle lording rates that are possible using molecular dynamics. This key issue of MD time scale (ns) vs. experimental fatigue time scale (s) is addressed in the present work using a combination of molecular statics and molecular dynamics. The combined results of these two techniques are shown to allow the basic understanding of the essential process of crack advance under cyclic loading. We will concentrate mostly on the behavior of Ni. The interatomic interactions for this material have been developed on the basis of first principles data [7] and tested as part of our previous work [8]. Using these potentials, we have previously studied realistic three dimensional polycrystalline samples of pure Ni under monotonic loading conditions. In this letter we report the first simulations under cyclic loading, performed on a digital sample with a columnar grain structure with random misorientations and a 6 nm grain size. Figure 1 shows the rates of crack advance as a function of stress intensity amplitude obtained from both molecular static and molecular dynamic simulations. These results are shown together with experimental results by Hanlon, Kwon and Suresh [10]. Figure 2 shows tip configurations after 26, and 31 cycles. Both configurations are at maximum loading, for the molecular statics simulations and a stress intensity amplitude of 1.4 MPa sqrt(m).

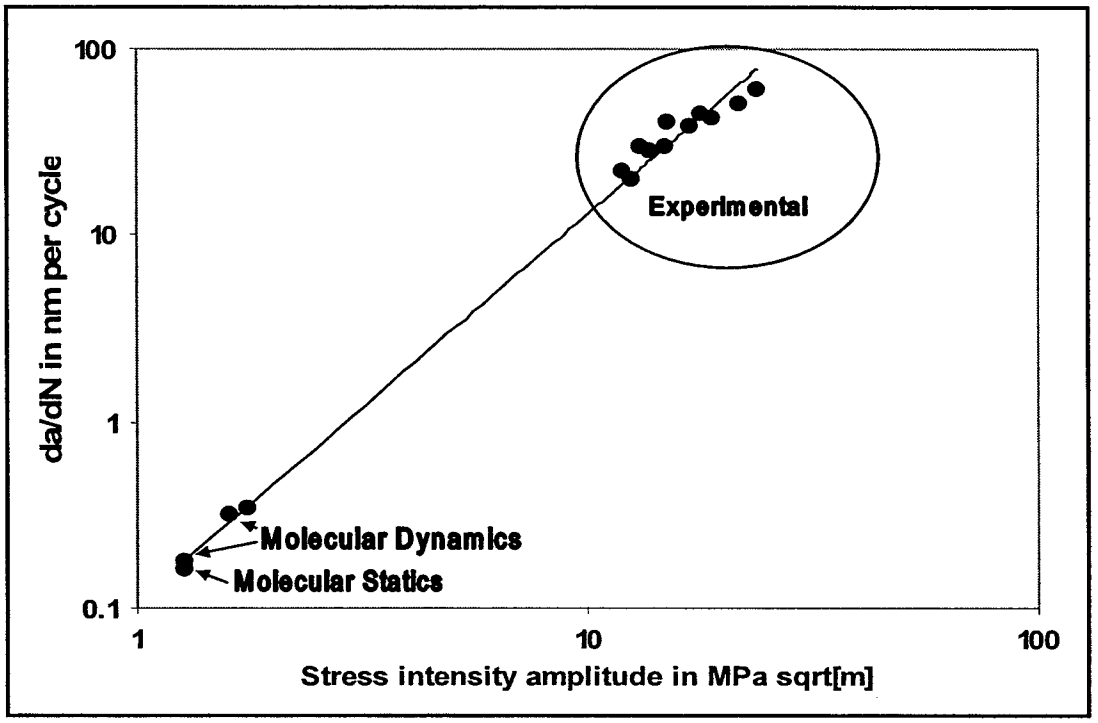

Figure 1: Resulting rate of crack advance for both molecular static and molecular dynamic simulations together with experimental results by Hanlon, Kwon and Suresh [10]

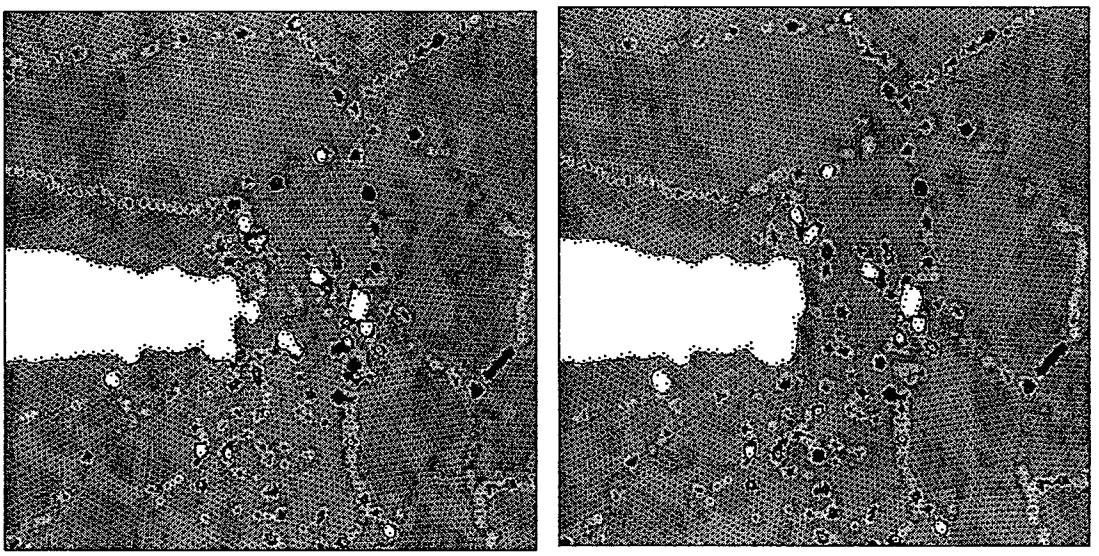

Figure 2: tip configurations after 26, and 31 cycles. Each picture is taken at maximum loading, for the simulations conducted using molecular statics and a stress intensity amplitude of 1.4 MPa sqrt(m).

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References

1. Kumar, KS; Van Swygenhoven, H; Suresh, S, Mechanical behavior of nanocrystalline metals and alloys, ACTA MATER, 51 (19): 5743-5774 NOV 25, 2003.

2. Weertman, JR; Farkas, D; Hemker, K; et al. , Structure and mechanical behavior of bulk nanocrystalline materials, MRS BULL, 24 (2): 44-50 FEB, 1999.

3. Deshpande, VS; Needleman, A; Van der Giessen, E, Scaling of discrete dislocation predictions for near-threshold fatigue crack growth,ACTA MATER, 51 (15): 4637-4651 SEP 3, 2003

4. Deshpande, VS; Needleman, A; Van der Giessen, E Discrete dislocation plasticity modeling of short cracks in single crystals, ACTA MATER, 51 (1): 1-15 JAN 8, 2003.

5. Deshpande, VS; Needleman, A; Van der Giessen, E, Discrete dislocation modeling of fatigue crack propagation, ACTA MATER, 50 (4): 831-846 FEB 25, 2002.

6. Deshpande, VS; Needleman, A; Van der Giessen, E , A discrete dislocation analysis of near-threshold fatigue crack growth, ACTA MATER, 49 (16): 3189-3203 SEP 20, 2001.

7. Mishin, Y; Farkas, D; Mehl, MJ; et al., Interatomic potentials for monoatomic metals from experimental data and ab initio calculations, PHYS REV B, 59 (5): 3393-3407 FEB 1 1999.

8. Farkas, D; Van Swygenhoven, H; Derlet, PM, Intergranular fracture in nanocrystalline metals, PHYS REV B, 66 (6): art. no.-060101 AUG 1, 2002

9. Van Swygenhoven, H; Spaczer, M; Caro, A; et al., Competing plastic deformation mechanisms in nanophase metals, PHYS REV B, 60 (1): 22-25 JUL 1 , 1999.

10. Hanlon, T; Kwon, YN; Suresh, S, Grain size effects on the fatigue response of nanocrystalline metals, SCRIPTA MATER, 49 (7): 675-680 OCT 2003.

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Publications

"ATOMISTIC MECHANISMS OF FATIGUE IN NANOCRYSTALLINE METALS" D. Farkas,
Mike Willemann and B. Hyde" to be submitted

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